Modeling of Surface Chemistry, Charge Transfer, and Transport in LSCF-Based Solid Oxide Fuel Cell Cathodes

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Establishing elementary chemical and electrochemical reaction pathways is one of the most difficult aspects of understanding the fundamental behavior of solid oxide fuel cell (SOFC) electrodes. One of the most powerful ways to achieve that is to use elementary kinetic numerical simulations.

The elementary kinetic model developed in the present work describes the electrochemical oxygen reduction at the LSCF/CGO based symmetrical SOFC system. The approach is based on (*i*) the elementary kinetic description of (electro-)chemical reactions [1], (*ii*) thermodynamically consistent reaction mechanism and (*iii*) physically meaningful surface potential step and electric potentials. For the mass transport model, two scales are taken into account, (*i*) porous gas-phase diffusion in the electrode using a coupled Fickian/Darcy transport mechanism and (*ii*) gas-phase transport in cathode channel above the electrode using a continuously stirred tank reactor (CSTR) model.

The simulation results are used to analyze experimental data, which were carried out using well-defined and thoroughly-characterized LSCF/CGO porous cathodes at different temperatures and microstructures [2]. Electrochemical impedance spectra were recorded for different atmospheres and temperatures at open circuit over a frequency range of 1 Hz - 1 MHz with a voltage stimulus of 10 mV [2]. Based on numerical impedance simulations [3], experimental data were successfully reproduced over the complete range of investigated gas compositions and operating temperatures. The three experimentally observed features of the impedance spectra were attributed to (*i*) gas diffusion in cathode channel, (*ii*) electrochemical oxygen reduction on the LSCF surface and incorporation into LSCF bulk, and (*iii*) charge-transfer of double negatively charged oxygen through two-phase boundary between LSCF and CGO. Two types of double layers (DL) were taken into account, that are, a surface DL formed by adsorbed negatively-charged oxygen ions on the LSCF surface and positively-charged sub-surface vacancies, and an interfacial DL at the contact between bulk LSCF and bulk CGO.

References

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